## **OCUMENTATION PAGE** REPOR AFRL-SR-AR-TR-03-Public reporting burden for this collection of information is estimated to average 1 hour per response, incligathering and maintaining the data needed, and completing and reviewing the collection of information. Sollection of information, including suggestions for reducing this burden, to Washington Headquarters Ser Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Pa of this Occal 2. REPORT DATE 1. AGENCY USE ONLY (Leave blank) 01 Aug 00 - 31 Jul 01 Final Report 13 Feb 02 5. FUNDING NUMBERS 4 TITLE AND SUBTITLE THE 2001 GORDON RESEARCH CONFERENCE ON MOLECULAR ENERGY F49620-00-1-0340 TRANSFER 2303/EX 6. AUTHOR(S) 61102F Mr Carlyle B. Storm 8. PERFORMING ORGANIZATION 7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) REPORT NUMBER Gordon Research Conferences Inc. P.O. Box 984 West Kingston, RI 02892-0984 10. SPONSORING/MONITORING 9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) AGENCY REPORT NUMBER AFOSR/NL 801 N Randolph Street, Suite 732 Arlington VA 22203-1977 11. SUPPLEMENTARY NOTES 12b. DISTRIBUTION CODE 12a. DISTRIBUTION AVAILABILITY STATEMENT Approve for Public Release: Distribution Unlimited 13. ABSTRACT (Maximum 200 words) The Gordon Research Conference (GRC) on Molecular Energy Transfer was held at Harbortown Resort, Ventura, California January 14-19, 2001. The conference was well attended with 89 participants (list enclosed). The attendees represented the spectrum of endeavor in this field coming from academia, industry, and government laboratories, both US and foreign scientists, senior researchers, young investigators, and students. In designing the formal speakers program, emphasis was placed on current unpublished research and discussion of the future target areas in this field. There was a conscious effort to stimulate lively discussion about the key issues in the field today. Time for formal presentations was limited in the interest of group discussions. In order that more scientists could communicate their most recent results, poster presentation time was scheduled. In addition to these formal interactions, "free time" was scheduled to allow informal discussions. Such discussions are fostering new collaborations and joint efforts in the field (program enclosed). 20030319 064 15. NUMBER OF PAGES 14. SUBJECT TERMS 16. PRICE CODE 18. SECURITY CLASSIFICATION | 19. SECURITY CLASSIFICATION | 20. LIMITATION OF ABSTRACT

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# GORDON RESEARCH CONFERENCES frontiers of science

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## 2001 GORDON RESEARCH CONFERENCE

on Molecular Energy Transfer



FINAL PROGRESS REPORT

AFOSR F49620-00-1-0340

The Gordon Research Conference (GRC) on Molecular Energy Transfer was held at Harbortown Resort, Ventura, California, January 14-19, 2001. The conference was well attended with 89 participants (list enclosed). The attendees represented the spectrum of endeavor in this field coming from academia, industry, and government laboratories, both US and foreign scientists, senior researchers, young investigators, and students.

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I want to personally thank you for your support of this Conference. As you know, in the interest of promoting the presentation of unpublished and frontier-breaking research, Gordon Research Conferences does not permit publication of meeting proceedings. If you wish any further details, please feel free to contact me. Thank you.

Joel Bowman Conference Chair

Approved for Public Release
Distribution Unlimited

## Molecular Energy Transfer

January 14-19, 2001 Harbortown Resort Ventura, CA



#### Contents:

- OVERVIEW, SPONSORS & SOCIAL PROGRAM
- PROGRAM
- POSTERS
- CONFERENCE HISTORY

#### Overview

As is customary, the meeting (which alternates every two years between Europe and the US) will cover all aspects of energy transfer, such as decomposition and reaction dynamics, intramolecular energy transfer, and energy transfer in media ranging from gas and clusters to condensed phases and interfaces. Several sessions will be devoted to new topics such as He nanodroplets, single molecule detection, etc. Oral sessions will take place in the morning and in the evening. At the beginning of each session, the session Chair will give a 20 minute perspective of the field. Each oral presentation will be 35 minutes, leaving ample time for discussion.

The conference will begin on Sunday afternoon at 4:30 PM with a reception and oral presentations at 7:30 PM. Poster sessions will take place after the evening talks on Monday - Thursday. Afternoons are free for discussions, volleyball at the beach, jogging, swimming, etc. Trips to nearby points of interest will be organized. The conference will culminate with the Thursday evening banquet, and the after dinner session in which the breadth of the field of molecular energy transfer, its modern practice and novel directions will be discussed. Departure is on Friday morning.

Application forms for the Gordon Conference must be submitted to the GRC office, P.O. Box 984, West Kingston, RI 02892-0984. Tel. 401 783-4011 (-7644 fax). Applications can also be made online by clicking the appropriate button at the bottom of this page. Early application is encouraged because the conference has usually close to the maximum allowed number of attendees. The deadline for registration at a reduced rate is 4 weeks prior to the conference. Please plan to apply by December 7, 2000. The deadline for submission of posters is December 22, 2000. We are trying to raise support for student and postdoc travel. The preliminary program is listed below. The full program with titles will be published in September.

#### Sponsors

- U.S. Air Force Office of Scientific Research
- · U.S. Office of Naval Research
- The Gordon Research Conferences
- · Gaussian, Inc.
- Spectra Physics
- Continuum Lasers

#### Social Program

#### Social Program

Tours to the Getty Museum and Whale Watching will be arranged for Tuesday afternoon. The cost will be about \$30 per trip. A sign-up sheet will be available on Sunday evening with more details.

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Somderson, Jennery 144, 2000						
2:00 - 9:00 p.m						
6:00 p.m.	Dinner					
	Spectroscopy and Reactivity in Clusters:					
	Session Chair: Marsha I. Lester					
7:30 - 7:40	Conference Chairs: Opening Remarks					
7:40 - 8:00	Marsha I. Lester (University of Pennsylvania) Perspective and overview					
8:00 - 8:50	Michael C. Heaven (Emory University) Non-adiabatic predissociation of Van der Waals molecules					
8:50 - 9:40	Nadine Halberstadt (Universite Paul Sabatier, Toulouse) Time-dependent study of vibrational energy relaxation in Van der Waals complexes: From the 1:1 diatomic-rare gas complex to the diatomic in a complete "solvent" shell					
<b>Μ</b> ήρουχεντικα	rement 15,2001. Unimateoria Reservoirs					
	Session Chair: Curt Wittig					
8:30	Conference Photo					
9:00 - 9:20	Curt Wittig: (University of Southern California) Perspective and overview					
9:20 - 10:10	Kaoru Yamanouchi (The University of Tokyo) Ultrafast structural deformation of small polyatomic molecules in intense laser fields					
10:10 - 10:40	Break					
10:40 - 11:30	Thomas R. Rizzo (Ecole Polytechnique Federale de Lausanne) IVR-limited unimolecular dissociation rates in state-selected HOCl and HOBr					
11:30 - 12:20	Reinhard Schinke (Max-Planck-Institüt fur Strömungsforschung) Quantum mechanical perspective of unimolecular dissociation					
12:30 - 1:30	Lunch					
2:00	Business Meeting					
Monthlylbine	January 15, 2000					
6:00 p.m.	Dinner					
	Photoussociation in Complexes					
	Session Chair: Jeremy M. Hutson					
7:30 - 7:50	Jeremy M. Hutson (University of Durham) Perspective and overview					
7:50 - 8:40	Robert E. Continetti (University of California at San Diego) Studies of three-body dissociation dynamics by dissociative dhotodetachment					
8:40 - 9:30	R. Benny Gerber (Hebrew University) Photochemical reactions, charge transfer and electronic energy relaxation in weakly-bound clusters					
9:30 p.m.	Poster Session I					
गाँगार सुन्धिकाणी	lamenty 10, 2001 Palpointhisponiciani de la laconomica de laconomica de la laconomica de la laconomica de la laconomica de					

	Session Chair: Keiji Morokuma
9:00 - 9:20	Keiji Morokuma (Emory University) Perspective and overview
9:20 - 10:10	Laurie J. Butler (The University of Chicago) Probing the dissociation dynamics of selected high-energy hydrocarbon radical isomers: Allyl, 1-propenyl and 2-propenyl
10:10 - 10:40	Break
10:40 - 11:30	Kirk A. Peterson (Washington State University) Photodissociation of halogen oxide molecules: HOCl, HOBr, and BrO
11:30 - 12:20	Jingsong Zhang (University of California, Riverside) Photodissociation dynamics of vinyl and ethyl radicals
12:30 - 1:30	Lunch
1:30 - 6:00 p.m	Optional Tours
Thestoypim.	Danvery (G.200)
6:00 p.m	Dinner
	He Namodroples
	Session Chair: Roger E. Miller
7:30 - 7:50	Roger E. Miller (University of North Carolina) Perspective and overview
7:50 - 8:40	Kenneth C. Janda (University of California, Irvine) Toward chemical reaction dynamics at 0.4 K
8:40 - 9:30	Andrej Vilesov (University of Southern California) Molecular spectroscopy in helium droplets
9:30 p.m.	Poster Session II
Wednesiky so	n. Jamen 17, 2001
Wednesikyzan	Bimolecular Reactions
Wednesday asi	
Wednesila, am 9:00 - 9:20	Bimolegylar Reactions
	Bimolecular Reactions Session Chair: Paul J. Dagdigian Paul J. Dagdigian (Johns Hopkins University)
9:00 - 9:20	Bimolecular Reactions Session Chair: Paul J. Dagdigian Paul J. Dagdigian (Johns Hopkins University) Perspective and overview Piergiorgio Casavecchia (Universita di Perugia)
9:00 - 9:20 9:20 - 10:10	Session Chair: Paul J. Dagdigian  Paul J. Dagdigian (Johns Hopkins University)  Perspective and overview  Piergiorgio Casavecchia (Universita di Perugia)  Recent progress in crossed beam studies of reaction dynamics  Break  David Manolopoulos (Oxford University)  Some recent developments in chemical reaction dynamics
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9:00 - 9:20 9:20 - 10:10 10:10 - 10:40 10:40 - 11:30 11:30 - 12:20 12:30 - 1:30	Session Chair: Paul J. Dagdigian  Paul J. Dagdigian (Johns Hopkins University)  Perspective and overview  Piergiorgio Casavecchia (Universita di Perugia)  Recent progress in crossed beam studies of reaction dynamics  Break  David Manolopoulos (Oxford University)  Some recent developments in chemical reaction dynamics  F. Javier Aoiz (Compluteuse University, Madrid)  A reaction with several paths: Dynamics and stereodynamics of the O(1D)+H2 reaction
9:00 - 9:20 9:20 - 10:10 10:10 - 10:40 10:40 - 11:30 11:30 - 12:20 12:30 - 1:30	Session Chair: Paul J. Dagdigian  Paul J. Dagdigian (Johns Hopkins University)  Perspective and overview  Piergiorgio Casavecchia (Universita di Perugia)  Recent progress in crossed beam studies of reaction dynamics  Break  David Manolopoulos (Oxford University)  Some recent developments in chemical reaction dynamics  F. Javier Aoiz (Compluteuse University, Madrid)  A reaction with several paths: Dynamics and stereodynamics of the O(1D)+H2 reaction  Lunch  Lunch  Dinner
9:00 - 9:20 9:20 - 10:10 10:10 - 10:40 10:40 - 11:30 11:30 - 12:20 12:30 - 1:30 Wednesday pure	Session Chair: Paul J. Dagdigian  Paul J. Dagdigian (Johns Hopkins University) Perspective and overview  Piergiorgio Casavecchia (Universita di Perugia) Recent progress in crossed beam studies of reaction dynamics Break  David Manolopoulos (Oxford University) Some recent developments in chemical reaction dynamics  F. Javier Aoiz (Compluteuse University, Madrid) A reaction with several paths: Dynamics and stereodynamics of the O(1D)+H2 reaction  Lunch  Lunch  January 1/2001  Dinner  Single-Molecule Studies of Energy I pansfer
9:00 - 9:20 9:20 - 10:10 10:10 - 10:40 10:40 - 11:30 11:30 - 12:20 12:30 - 1:30 Wednesday pure	Session Chair: Paul J. Dagdigian  Paul J. Dagdigian (Johns Hopkins University)  Perspective and overview  Piergiorgio Casavecchia (Universita di Perugia)  Recent progress in crossed beam studies of reaction dynamics  Break  David Manolopoulos (Oxford University)  Some recent developments in chemical reaction dynamics  F. Javier Aoiz (Compluteuse University, Madrid)  A reaction with several paths: Dynamics and stereodynamics of the O(1D)+H2 reaction  Lunch  Lunch  Dinner
9:00 - 9:20 9:20 - 10:10 10:10 - 10:40 10:40 - 11:30 11:30 - 12:20 12:30 - 1:30 Wedinesday pol 6:00 p.m.	Session Chair: Paul J. Dagdigian  Paul J. Dagdigian (Johns Hopkins University) Perspective and overview  Piergiorgio Casavecchia (Universita di Perugia) Recent progress in crossed beam studies of reaction dynamics Break  David Manolopoulos (Oxford University) Some recent developments in chemical reaction dynamics  F. Javier Aoiz (Compluteuse University, Madrid) A reaction with several paths: Dynamics and stereodynamics of the O(1D)+H2 reaction  Lunch  Lunch  Limitary 17, 2001  Dinner  Single-Molceule Studies of Energy Transfer Session Chair: George W. Flynn  George W. Flynn (Columbia University)
9:00 - 9:20 9:20 - 10:10 10:10 - 10:40 10:40 - 11:30 11:30 - 12:20 12:30 - 1:30 Wedinesday par 6:00 p.m.	Session Chair: Paul J. Dagdigian  Paul J. Dagdigian (Johns Hopkins University)  Perspective and overview  Piergiorgio Casavecchia (Universita di Perugia)  Recent progress in crossed beam studies of reaction dynamics  Break  David Manolopoulos (Oxford University)  Some recent developments in chemical reaction dynamics  F. Javier Aoiz (Compluteuse University, Madrid)  A reaction with several paths: Dynamics and stereodynamics of the O(1D)+H2 reaction  Lunch  Lunch  Lunch  Single-Molecule Studies of Energy Transfer  Session Chair: George W. Flynn  George W. Flynn (Columbia University)  Perspective and overview  Paul F. Barbara (University of Texas, Austin)

9:30 p.m.

Poster Session III

9:30 p.m.	POSTGI DESSION III
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	Intercy Henrice Condensed Press.
	Session Chair: Peter J. Rossky
9:00 - 9:20	Peter J. Rossky (University of Texas, Austin) Perspective and overview
9:20 - 10:10	Gilbert M. Nathanson (University of Wisconsin, Madison) One second in the life of HCl in liquid glycerol: Solvation, dissociation, and recombination
10:10 - 10:40	Break
10:40 - 11:30	Stephen E. Bradforth (University of Southern California) The dynamics of photodetachment and photoionization in aqueous solution
11:30 - 12:20	Tim Lian (Emory University) Dynamics of molecular adsorbates on nanoparticles: vibrational relaxation, solvation and electron transfer
12:30 - 1:30	Lunch
4:00 - 6:00 p.m	Poster Session IV
Manastery jum	Jamuary 18, 2000
6:00 p.m.	Dinner
	New Tirends in Molecular Energy Draister.
	Session Chair: Millard H. Alexander
8:00 - 8:20	Millard H. Alexander (University of Maryland) Perspective and overview
8:20 - 9:20	Stephen R. Leone (NIST/University of Colorado)  Molecular energy transfer - where are we going? From vibration-vibration to quantum information science
9:20 - 9:30	Conference Chairs: Summary Comments
ir dayara ji	mnerry 19, 200 t
7:30 - 8:30	Breakfast
9:00:	End of Conference; Bus Departs

#### Poster Sessions I and II: Displayed Monday and Tuesday

Odd numbers: Presented Monday Even numbers: Presented Tuesday

- Experimental Investigation of the Low Lying Electronic States of CH<sub>2</sub>Cl
   <u>Aaron Potter</u>, <u>Vladimir Dribinski</u>, Andrey Demyanenko and Hanna Reisler Chemistry Department, University of Southern California
- Laser Jet Spectroscopy of Molecular Microclusters of Pyridylindoles
  Y. Nosenko and A. Mordzinski
  Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw
- Ab Initio Calcluations of Electronically Excited States of the CH<sub>2</sub>Cl Radical <u>S. Levchenko</u> and A. Krylov. Chemistry Department, University of Southern California
- 4. The Infrared Spectroscopy of H-Bonded Dimers in their Ground and First Excited Singlet States Gina M. Florio, Edwin L. Sibert, III, Christopher J. Gruenloh, and Timothy S. Zwier

Purdue University, West Lafayette, IN and University of Wisconsin-Madison

- Infrared Spectroscopy of Vibrationally Excited Methanol and Some of its Isotopomers
   <u>D. Rueda</u>, O. V. Boyarkin, T. R. Rizzo
   Laboratoire de Chimie Physique Moléculaire, EPFL, Lausanne
   A. Chirokolava, D. S. Perry
   Department of Chemistry, University of Akron, Ohio
- Vibrationally Mediated Photodissociation of H<sub>2</sub>O
   <u>Joelle Underwood</u>, Delphine Chastaing, Judson Partin, and Curt Wittig
   Chemistry Department, University of Southern California
- Photodissociation Dynamics of CH<sub>2</sub>OH and its Isotopomers from the 3p<sub>z</sub> Rydberg State <u>Feng. L</u>; Khodykin, O; Conroy D; Aristov, V; Nishimura. P; Reisler, H Chemistry Department, University of Southern California
- Mapping of the OH + CO reaction pathway throught infrared spectroscopy of the OH-CO reactant complex
   <u>Marsha Lester</u>, Bethany V. Pond, Mark D. Marshall, and David T. Anderson,
   Department of Chemistry, University of Pennsylvania
   Lawrence B. Harding and Albert F. Wagner,
   Chemistry Division, Argonne National Laboratories
- Dynamics of vibrationally mediated photodissociation of H<sub>2</sub>O and Ar-H<sub>2</sub>O, <u>Sergey A. Nizkorodov</u>, Michael Ziemkiewicz, Tanya L. Myers, David J. Nesbitt. <u>JILA/NIST</u> and Department of Chemistry and Biochemistry, University of Colorado,
- Emission Spectroscopy and Ab Initio Characterization of the Excited States of Allyl Iodide and Allyl Alcohol Accessed Near 200 nm
   <u>Brad Parsons</u> and Laurie J. Butler
   Department of Chemistry, The University of Chicago
- Ab initio calculation of widths of HOCl(7v<sub>OH</sub>, and 8v<sub>OH</sub>) resonances and comparison with experiment.
   Shengli Zou, Sergei Skokov, and Joel M. Bowman
   Cherry L. Emerson Center for Scientific Computation and Dept. of Chemistry, Emory University
- QUASICLASSICAL TRAJECTORY STUDY OF THE H (Cl) + HCN --> H<sub>2</sub> (HCl) + CN REACTION DYNAMICS AND MICROSCOPIC MECHANISM
   Diego Troya <sup>(a)</sup>, Miguel González <sup>(b)</sup> \*, Guosheng Wu <sup>(c)</sup>, and George C. Schatz <sup>(c)</sup> \*
   (a) Departamento de Química, Universidad de La Rioja,
   C/ Madre de Dios, 51. 26004 Logroño (Spain).
   (b) Departament de Química Física i Centre de Recerca en Química Teòrica,
   Universitat de Barcelona, C/ Martí i Franquès, 1. 08028 Barcelona (Spain).
   (c) Departament of Chemistry, Northwestern University, 2145 Sheridan Rd,
   Evanston IL 60208-3113 (USA).
- 13. NASCENT OH(X<sup>2</sup>Π;, v"=0-4) STATE-DISTRIBUTIONS FROM THE O(<sup>1</sup>D)+C<sub>2</sub>H<sub>6</sub>, C<sub>2</sub>H<sub>4</sub>
  REACTIONS. A LIF AND QCT STUDY
  Miguel González (a) \*, María P. Puyuelo (b), Jordi Hernando (a), R. Sayós (a), Pedro A. Enríquez (b), and Javier Guallar (b)
  (a) Departament de Química Física i Centre de Recerca en Química Teòrica,
  Universitat de Barcelona, C/ Martí i Franquès, 1. 08028 Barcelona (Spain)
  (b) Departamento de Química, Universidad de La Rioja,
  C/ Madre de Dios, 51. 26004 Logroño (Spain)
- Semiclassical Tunneling Splitting of the Ground State
   <u>Gennady Mil'nikov</u> and H. Nakamura
   Department of Theoretical Studies, Institute for Molecular Science, Okazaki, Japan.

- 15. The Vibrational Energy Transfer of NO(X<sup>2</sup>Π, v) to NO<sub>2</sub>(v<sub>3</sub>) Studied by Tme-Resolved FTIR Emission Spectroscopy Yuchuan Gong, Xiron Chen, and Brad R. Winer Department of Chemistry, University of Puerto Rico, San Juan
- 16. Unimolecular Reaction Rate Constants of NO<sub>2</sub> Just Above the Treshold <u>Daniil Yu Stolyarov</u> and Curt Wittig University of Southern California
- Absolute Cross Sections for Vibrational Deactivation and Electronic Quenching of the pDFB molecule
  with High Vibrational Energy
  <u>Uros S. Tasic</u> and C. Parmenter
  Department of Chemistry, Indiana University
- 18. Collisional Energy Transfer of Highly Vibrationally Excited Methyl- and Azabenzenes: Transition Probabilities and Relaxation Pathways from KCSI Experiments and Trajectory Calculations Uwe Grigoleit, Thomas Lenzer, <u>Klaus Luther</u>, Martin Muetzel, and Atsuko Takahara Institut fuer Physikalische Chemie, Universitat Goettingen, Germany
- The H + NO<sub>2</sub> Channels in the Photodissociation of HONO at 193.3 nm Gabriel Amaral, <u>Kesheng Xu</u> and Jingsong Zhang Department of Chemistry, University of California, Riverside
- Site-specific Photodissociation of Ethyl Iodide at 193.3 nm <u>Gabriel Amaral</u>, Kesheng Xu and Jingsong Zhang Department of Chemistry, University of California, Riverside
- Predominance of Non-Equilibrium Dynamics in the Photodissociation of Ketene in the Triplet State
   <u>A.L. Kaledin</u>, J. Seong, and K. Morokuma
   Cherry L. Emerson Center for Scientific Computation and Dept. of Chemistry, Emory University
- Potential energy surfaces for the A<sup>2</sup> A state of CH-Ar <u>Galina Y. Kerenskaya</u>, Alexey L. Kaledin, and Michael C. Heaven Department of Chemistry, Emory University, Atlanta
- Kinetic spectroscopy of NCl
   A. V.Komissarov, M. C. Heaven
   Department of Chemistry, Emory University, Atlanta
- Dynamics of Rovibrational Transfer in Li<sub>2</sub>-Ne Collisions
   Kristin M. Burgess, Amy M. Schneider, Troy N. Stephens, Alena Widman, and Brian Stewart Chemistry Department, Wesleyan University
- 25. The photodissociation of CH<sub>3</sub>SCH<sub>3</sub> and CD<sub>3</sub>SCD<sub>3</sub> in the first absorption band studied by velocity map imaging and REMPI F. J. Aoiz, <sup>1</sup> L. Banares, <sup>1</sup> B. Martinez-Haya, <sup>2</sup> P. Quintana, <sup>1</sup> and E. Verdasco <sup>1</sup> 1. Departamento de Quimica Fisica, Facultad de Quimica and CAI de Espectroscopia. Universidad Comlutense. 28040 Madrid, Spain 2. Departamento de Ciencias Ambientales, Facultad de Ciencias Experimentales, Universidad Pablo de Olavide, Ctra. de Utrera, km, 1, 1013 Sevilla, Spain
- Combining hexapoles with stimulated emission pumping.
   Daniel Matsiev, and <u>Alec M. Wodtke</u>
   UC Santa Barbara, Department of Chemistry & Biochemistry, Santa Barbara, CA
- Spectra of water dimer and trimer from ab initio potentials
   <u>Krzysztof Szalewicz</u>
   Department of Physics and Astronomy, University of Delaware

- Electronic Spectroscopy and State-Resolved Photodissociation of Jet-Cooled Vinyl Radical <u>M.B. Pushkarsky</u>, A. Mann and C. B. Moore Laser Spectroscopy Facility, Dpartment of Chemistry, The Ohio State University
- 29. Jeremy Hutson
- 30. John Mccaffrey

### Poster Sessions III and IV: Displayed Wednesday and Thursday

Odd numbers: Presented Wednesday Even numbers: Presented Thursday

- Low-temperature kinetics of reactions of C<sub>2</sub>H and OH radicals with selected hydrocarbons
   <u>A. B. Vakhtin</u>, S. Lee, D. E. Heard(\*), I. W. M. Smith(\*), and S. R. Leone
   JILA, NIST and University of Colorado, Department of Chemistry and Biochemistry
   (\*) JILA Visiting Fellow
- Photodissociation of ICN in Cyclohexane: A Study of Solvent Effects on Reaction Dynamics
   <u>Amy C. Germaine</u>, Victor A. Lenchenkov, Victor H. Vilchiz, Jeremiah A. Kloepfer, and Stephen E.
   Bradforth
   Chemistry Department, University of Southern California
- Rotationally Inelastic Collisions of Highly Rotationally Excited Free Radicals: CH(A<sup>2</sup>Λ) and CN(A<sup>2</sup>Π)
   B.Nizamov and P.J. Dagdigian.
   Chemistry Department, The Johns Hopkins University
- Femtosecond Dynamics of ICl (CO<sub>2</sub>)<sub>n</sub> Clusters
   <u>Django Andrews</u> and Carl Lineberger
   JILA, University of Colorado, Boulder, Colorado
- Dynamics of Harpooning in Li..FCH<sub>3</sub> van der Waals complex
   A.J. Hudson, F.Y. Naumkin, H.B. Oh, <u>S.R. Raspopov</u> and J.C. Polanyi Department of Chemistry, University of Toronto
- 6. Inter- and intramolecular energy transfer of diphenylpolyenes in solution explored by fs-fluorescence up-conversion.
   C. Grimm, J. Schroeder, <u>T. Steinel</u> and J. Troe IPC, University of Goettingen
- Theoretical studies of the product translational energy distributions in the F + HD --> HF + D reaction <u>Yi-Ren Tzeng</u> and Millard H. Alexander Department of Chemistry and Biochemistry and Chemical Physics Program, University of Maryland
- Vibrational Self-consistent Field Approach to Anharmonic Spectroscopy of Molecules in Solids: Application to I<sub>2</sub> in Argon Matrix
   Zsolt Bihary, Benny Gerber, and Ara Apkarian University of California, Irvine, USA and Hebrew University, Israel
- Comparison of the Reactivity of the Symmetric and Antisymmetric Stretch of CH<sub>4</sub> on the Reaction of Cl
   (<sup>2</sup>P<sub>3/2</sub>) + CH<sub>4</sub>
   Sangwoon Yoon, Sarah Henton, Aleks Zivkovic, and F. Fleming Crim
   Department of Chemistry, University of Wisconsin-Madison
- Full-dimensional IVR calculations on medium-sized organic molecules and their comparison to experiment: Pyrrole and Triazine.
   Ryan Pearman and Martin Gruebele
   Department of Chemistry, University of Illinois

- The effect of Ar atoms on the dynamics of the O(<sup>3</sup>P) + HCl reaction <u>Lichang Wang</u>, and Anne B. McCoy Department of Chemistry, The Ohio State University
- 12. Time-resolved studies of energy transfer from a vibrationally excited I<sub>2</sub>- chromophore into surrounding Ar or CO<sub>2</sub> clusters

  Reland Wester, Alicen V. Davis, Arthur F. Bragg, Daviel M. Neumark

Roland Wester, Alison V. Davis, Arthur E. Bragg, Daniel M. Neumark Department of Chemistry, University of California, Berkeley

- 13. Reduced dimensionality quantum calculations of the Cl + CH<sub>4</sub> reaction and a prediction on the effect of bend excitation on the HCl rotational distribution.
  Sergei Skokov and <u>Joel M. Bowman</u>
  Cherry L. Emerson Center for Scientific Computation and Dept. of Chemistry, Emory University,
- 14. THEORETICAL STUDY OF THE N(<sup>4</sup>S) + O<sub>2</sub>(X<sup>3</sup>Σ<sub>g</sub><sup>-</sup>) --> NO(X<sup>2</sup>Π) + O(<sup>3</sup>P) REACTION. FROM THE ELECTRONIC STRUCTURE TO THE RATE CONSTANT. Carolina Oliva, Miguel González, and R. Sayós Departament de Química Física i Centre de Recerca en Química Teòrica C/ Martí i Franqués 1, Barcelona (Spain)
- 15. Ab initio <sup>3</sup>A" ground potential energy surface for the O(<sup>3</sup>P) + N<sub>2</sub>O reaction and kinetics study Rosendo Valero, R. Sayós, and Miguel González Departament de Química Física i Centre de Recerca en Química Teòrica, Universitat de Barcelona. C/ Martí i Franquès, 1. 08028 Barcelona, Spain.
- 16. Ab initio and VTST kinetics study of the N(¹D)+O<sub>2</sub>(X³Σ<sub>g</sub>) reaction including excited PES Irene Miquel, R. Sayós \*, and Miguel González \* Departament de Química Física i Centre de Recerca en Química Teòrica, Universitat de Barcelona. C/ Martí i Franquès, 1. 08028 Barcelona, Spain.
- Vibrational spectroscopy and intermolecular vibrational energy transfer for glycine molecule and its complex with water.
   Galina M. Chaban, R. Benny Gerber
   NASA Ames Research Center, Moffett Field, CA, and Hebrew University, Israel
- Relaxation Processes in Multimolecular Systems
   <u>Eduard Zenkevich</u>
   Laboratory of Molecular Photonics, Institute of Molecular and Atomic Physics, Minsk, Belarus
- NO(v)-O vibrational energy transfer and its photochemical role in the thermosphere
   <u>Eunsook S. Hwang<sup>1</sup></u> and James Dodd<sup>2</sup>
   (1)Stewart Radiance Laboratory, Bedford, MA, and (2) Air Force Research Lab, Hanscom AFB
- Recent Studies of OH(v) Dynamics
   <u>James A. Dodd</u><sup>1</sup> and Eunsook S. Wang<sup>2</sup>
   (1) Air Force Research Laboratory, Hanscom AFB, MA; and Stewart Radiance Laboratory, Bedford, MA
- Quantum Dynamical Studies of Atom-Diatom Insertion Reactions <u>Jean-Michel Launay</u> and Pascal Honvault Université de Rennes, UMR 6627 du CNRS, Rennes, France
- Li + HF: A Case Study to Develop Novel Computational Technologies for Reactive Scattering
   <u>Antonio Lagana</u>
   Universita di Perugia, Dipartimento di Chimica, Italy
- 23. Theoretical Study of Scanning tunneling Miscroscope Induced Desorption of Benzene from Si(100)

Surface
Saman Alavi, Roger Rousseau and Tamar Seideman
National Research Council of Canada, Steacie Institute for Molecular Sciences, Ottawa, Canada

- Isotopically Selective Collisonal Vibrational Energy Transfer Oleg Boiarkine and T.R. Rizzo EPFL, LCPM, DC. EPFL, Lausanne, Switzerland
- 25. The Relavative Distributions of State-to-State Inelastic Scattering Cross Sections of S<sub>1</sub> trans-Glyoxal Demonstrate a Center-of-Mass Momentum Correlation Samuel M. Clegg, Mariana Duca and Charles S. Parmenter Sandia National Laboratories, Livermore, CA
- 26. The Dynamics and Stereodynamics of Four-Body Chjemical Reactions by Quasiclassical Trajectory Methods on Ab Initio Potential Energy Surfaces <u>Jesus Santamaria</u> Universidad Complutense de Madrid, Departamento de Quimica Fisica, Facultad de Quimica, Madrid, Spain
- 27. Energy transfer from excited NH<sub>2</sub> in the presence of NO, studied by time-resolved FTIR emission spectroscopy <u>Timothy P. Marcy</u>, Dwayne E. Heard and Stephen R. Leone JILA/NIST and Department of Chemistry and Biochemistry, University of Colorado
- 28. Trajectory Surface-Hopping Study of the  $I(^2P_{3/2}) + O_2(a^1\Delta_g) --> I(^2P_{1/2}) + O_2(X^3\Sigma_g)$  Energy Transfer Process A.L. Kaledin, M.C. Heaven, and K. Morokuma Cherry L. Emerson Center for Scientific Computation and Dept. of Chemistry, Emory University
- A quasi-classical trajectory study of the H+N<sub>2</sub>O reaction
   J. F. Castillo, F. J. Aoiz, <u>L. Banares</u>, and J. Santamaria
   Departamento de Quimica Fisica, Facultad de Quimica and CAI de Espectroscopia. Universidad Comlutense. 28040 Madrid, Spain
- New 3-D potential energy surface for the He-CO system
   George C. McBane and Kirk Peterson
   Department of Chemistry, The Ohio State University and Washington State University
- 31. Vibrational effects in collision-induced dissociation dynamics of the Ar<sub>2</sub>+ + Ar/Ne systems
   J. Scott Miller, <sup>1</sup> Rainer Dressler, <sup>1</sup> Yu-hui Chiu, <sup>2</sup> and Dale J. Levandier<sup>2</sup>
   (1) Air Force Research Lab, Hanscom AFB, and (2) Boston College, Institute of Scienctific REsearch, Newton.

### **Conference History**

Continuing progress in our understanding of molecular energy transfer, and the importance of this process, have provided the impetus for a series of conferences on this topic, dating back to 1969. The conferences have taken place biennially, in alternation between a Gordon Research Conference (GRC) on Molecular Energy Transfer and a European Conference on Molecular Energy Transfer (COMET). This alternation underlines the international aspect of the field and provides a regular channel for exchange between scientists in North America and Europe. The previous GRC/COMET conferences in this series, sites, and organizers are listed below.

Date	Conference	Site	Conference Chair(s)
969	CRCT .	New Hampshire	Patiney-Stemical and Charles Patimenter
971	COME	Cambridge (UK)	Anthony Galleric .
97/3	GROUP S	Way Hampshire - Wes	C. Brasley Moore
975	COMIN	Logann (Generaly)	Parastoninies .
977	GRC 1	New Hampsing	George Hyan
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9812	GRC -	New Lampsbire	Thomas Score .
983	COME	Giren (esto: (IUK))	Anthony McCaffery
985	GRC 10	New Plampshits	Paul Housion and Stephen Leone.
987	COMIDI	Emmerica (Style/Mand):-	Maridin Quade y
980	GRC T	New Hampshire	Ente Weitz and George Schatz
90)	COMM	Riffregan (Matierales)	lioig Repiss
993¥	JORC - 4	- New Hampshire	David Kingand John Stephenson
995	COMER	Z Kulosier Bahy (Germany)	Hans-loachin Wemerand Reter Andresen:
997*	GRO I	Venina, CA	Marsina Lesier and Millard Allexander
009	COMETA	Ajraky	Amonio Lagaria and P. Casavecchia
0014	GRE	A Vennes CAC.	i Banna Reisler and Joek Bownan.
2003	COMET	Spain 2	R Java: Adizand Migual Gonzalez



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# MOLECULAR ENERGY TRANSFER

FOUR POINTS SHERATON: HARBORTOWN (14-Jan-01) - (19-Jan-01)

NOTE: Receipt of Application does not guarantee acceptance to a Conference. Applications are reviewed by the Conference Chair. If the Chair approves your application, you become Accepted, and a registration packet will be mailed immediately. Please allow 3-5 days for your registration to reach you by mail once your name appears. When your registration packet has been received back in our office, you become Registered.

Only those who have been Accepted or Registered will have their names listed below. Names of people who have only applied and have yet to be accepted will NOT appear.

Name	Organization	Participation	
SAMAN ALAVI	NATIONAL RESEARCH COUNCIL OF CANADA	Poster Presenter	Registered
MILLARD H ALEXANDER	UNIVERSITY OF MARYLAND	Speaker	Registered
DJANGO H ANDREWS	UNIVERSITY OF COLORADO	Poster Presenter	Registered
FRANCISCO J AOIZ	UNIVERSIDAD COMPLUTENSE	Speaker	Registered
LUIS BANARES	UNIVERSIDAD COMPLUTENSE	Poster Presenter	Registered
PAUL F BARBARA	UNIVERSITY OF TEXAS AT AUSTIN	Speaker	Registered
ZSOLT BIHARY	UNIVERSITY OF CALIFORNIA	Poster Presenter	Registered
OLEG V BOLARKINE	SWISS FED. INSTIT. OF TECH.	Poster Presenter	Registered
JOEL BOWMAN	EMORY UNIVERSITY	Chair	Registered
STEPHEN E BRADFORTH	UNIVERSITY OF SOUTHERN CALIFORNIA	Speaker	Registered
LAURIE J BUTLER	THE UNIVERSITY OF CHICAGO	Speaker	Registered
PIERGIORGIO CASAVECCHIA	UNIVERSITA DI PERUGIA	Speaker	Registered
GALINA M CHABAN	NASA	Poster Presenter	Registered
STEVE CHAMBREAU	UNIVERSITY OF CALIFORNIA, RIVERSIDE	Poster Presenter	Registered
DELPHINE CHASTAING	UNIVERSITY OF SOUTHERN CALIFORNIA	Attendee	Registered
	SANDIA NATIONAL LABORATORIES	Poster Presenter	Registered
SAMUEL M CLEGG ROBERT E CONTINETTI	UNIV. OF CALIFORNIA, SAN DIEGO	Speaker	Registered
	JOHNS HOPKINS UNIVERSITY	Speaker	Registered
PAUL J DAGDIGIAN	AIR FORCE RESEARCH LABORATORY	Poster Presenter	Registered
JAMES A DODD	UNIVERSITY OF SOUTHERN CALIFORNIA	Poster Presenter	Registered
VLADIMIR L DRIBINSKI	UNIVERSITY OF SOUTHERN CALIFORNIA	Poster Presenter	Registered
LIN FENG	PURDUE UNIVERSITY	Poster Presenter	Registered
GINA M FLORIO	COLUMBIA UNIVERSITY	Speaker	Registered
GEORGE W FLYNN	HEBREW UNIVERSITY	Speaker	Registered
BENNY GERBER	UNIVERSITY OF SOUTHERN CALIFORNIA	Poster Presenter	Registered
AMY C GERMAINE	UNIVERSITY OF PUERTO RICO	Poster Presenter	Registered
YUCHUAN GONG	UNIVERSITY OF BARCELONA	Poster Presenter	Registered
MIGUEL GONZALEZ	CNRS-UNIVERSITE PAUL SABATIER	Speaker	Registered
NADINE HALBERSTADT	UNIVERSITY OF CALIFORNIA, SANTA BARBARA	Attendee	Registered
NILS HANSEN	EMORY UNIVERSITY	Speaker	Registered
MICHAEL C HEAVEN	UNIVERSITY OF CALIFORNIA	Speaker	Registered
WILSON HO	UNIVERSITY OF DURHAM	Speaker	Registered
JEREMY M HUTSON	UTAH STATE UNIVERSITY	Poster Presenter	Registered
EUNSOOK S HWANG	UNIVERSITY OF CALIFORNIA, IRVINE	Speaker	Registered
KENNETH C JANDA	EMORY UNIVERSITY	Poster Presenter	Registered
ALEXEY L KALEDIN	EMORY UNIVERSITY	Poster Presenter	Registered
GALINA KERENSKYA	EMORY UNIVERSITY	Poster Presenter	
ANATOLY V KOMISSAROV	UNIVERSITE DE RENNES	Poster Presenter	Registered
JEAN-MICHEL LAUNAY	NIST/ UNIVERSITY OF COLORADO	Speaker	Registered
STEPHEN LEONE	UNIVERSITY OF PENNSYLVANIA	Speaker	Registered
MARSHA I LESTER	BOSTON COLLEGE INSTITUTE FOR SCIENTIFIC RESEARCH	Poster Presenter	Registered
DALE J LEVANDIER	UNIVERSITY OF SOUTHERN CALIFORNIA	Poster Presenter	Registered
SERGEY V LEVCHENKO	EMORY UNIVERSITY	Speaker	Registered
TIANQUAN LIAN	UNIVERSITY OF COLORADO, BOULDER	Attendee	Registered
CARL LINEBERGER	UNIVERSITI OF COLORADO, DOUBDER		-

Registered

Attendee

KLAUS H LUTHER DAVID MANOLOPOULOS TIMOTHY P MARCY DANIEL V MATSIEV GEORGE C MCBANE JOHN MCCAFFREY ANNE B MCCOY ROGER E MILLER ANDRZEJ MORDZINSKI KEIJI MOROKUMA GILBERT M NATHANSON **BORIS R NIZAMOV** SERGUEI A NIZKORODOV CHARLES PARMENTER BRADLEY F PARSONS RYAN PEARMAN KIRK A PETERSON ELENA YU POLYAKOVA AARON B POTTER MICHAEL B PUSHKARSKY SERGUEI A RASPOPOV HANNA REISLER THOMAS R-RIZZO PETER J ROSSKY DAVID RUEDA REINHARD SCHINKE TOBIAS STEINEL BRIAN A STEWART DANIIL YU STOLYAROV KRZYSZTOF SZALEWICZ UROS S TASIC YI-REN TZENG JOELLE S UNDERWOOD ANDREI VAKHTIN MARC C VAN HEMERT ANDREJ VILESOV LICHANG WANG **ROLAND WESTER CURT WITTIG** ALEC WODTKE KESHENG XU KAORU YAMANOUCHI SANGWOON YOON JINGSONG ZHANG

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